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ORIGINAL PAPER

George M. Frame

A collaborative study of 209 PCB congeners and 6 Aroclors on 20 different HRGC columns

1. Retention and coelution database

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Abstract The elution orders and predicted coelutions of all 209 PCB congeners were obtained for 27 HRGC-ECD or HRGC-MS systems comprising 20 different stationary phases. The resultant database facilitates selection of the columns most suitable for developing particular comprehensive, quantitative, congener-specific PCB analyses, the design of the minimum number of congener mixtures needed to calibrate such analyses, and the testing of retention prediction algorithms based on structure relationships of GC phases and congener substitution patterns.

Introduction

Polychlorinated biphenyls (PCBs) in samples analyzed for environmental and regulatory purposes usually consist of complex mixtures of up to half or more of the 209 possible different chlorine-substituted biphenyl congeners, derived from technical mixtures (e.g. Aroclors [1, 2], Clophens, Kanechlors etc.). Additional congeners may be encountered in samples where processes such as photolytic, microbial, thermal or chemical dechlorination, or metabolism in higher animals have acted upon the initial distribution in a technical mixture [3]. Regulatory analysis requirements are sometimes limited to quantitation as total amount of PCB [4], as amounts of specific technical mixture distributions [5], or as separate amounts of specified small subsets of individual priority congeners [6, 7].

G. M. Frame
Environmental Laboratory,
GE Corporate Research and Development Center, Bldg. K1,
Rm 3B32, P.O. Box 8, Schenectady, NY, 12301–0008, USA

Supplementary material The retention database for all 27 systems, both in the form of Table 2, and ordered by IUPAC number, the RRF database for all systems ordered by IUPAC number, a listing of the 9 proposed congener calibration mixes and a table of elution orders and relative separations of PCBs in each of them for all systems, and copies of Tables 1A and 1B, are available over the World Wide Web as Excel 4.0 files, ASCII data files, and in Adobe Acrobat PDF format through the Fresenius' Journal home page using URL http://science.springer.de/fjac/fjac.htm.

Many research applications, particularly those investigating the alteration processes listed above, require comprehensive, quantitative, congener-specific (CQCS) analyses.

The methods of choice for many of the regulatory as well as CQCS analyses employ high resolution gas chromatography (HRGC) on capillary columns with selective, sensitive detection by electrolytic conductivity detectors (ELCD), electron capture detectors (ECD) or selected-ion-monitoring mass spectrometry (MS-SIM). CQCS analyses by HRGC are defined here as those in which the goal is to have all congeners present correctly assigned to the peaks in which they elute, and to quantify the PCB content in each resolved peak against an appropriate standard. When MS-SIM detection is used, coeluting PCB congener homologs of differing chlorine number may sometimes be separately quantified as well. Larsen has recently provided a lengthy and comprehensive review of the HRGC separation of PCB congeners [6]. No single column can resolve all 209 congeners, or even all those typically encountered in applications requiring CQCS methods. Larsen's laboratory has identified columns (series coupled HT-5/DB-5 [8, 9], HT-5 [10, 11], and HT-8 [12]) with favorable resolution performance for quantitating specific subsets [6, 7], and these papers describe the elution of many additional congeners on these columns. Elution orders for all 209 congeners have been published for an SE-54 capillary [13], the non-polar Chrompack CP-Select for PCBs capillary [14], and the 007-ODP (40% octadecyl-, 15% phenyl, methyl-silicone) phase [15]. Extensive congener assignments have been made to peaks from Aroclor mixtures eluting from highly polar Sil-88 (50% cyanopropyl-, 50% phenyl- polysiloxane) [11], as well as to capillary columns coated with phases equivalent to those discussed in this paper [1, 9, 11, 12, 13, 15, 16, 17, 18, 19, 20, 21, 22; cf, Table 1A].

In earlier years most analysts did not have ready access to standards of all 209 PCB congeners to assign them to HRGC peaks and to calibrate CQCS analyses. More commonly, technical mixtures (usually Aroclors) were employed, and peak assignments for unavailable congeners were estimated by a variety of quantitative structure-activity relationship models [6, 14, 23, 24, 25, 26]. These were sometimes sufficient to provide a correct assignment, but none consistently predicted retention times to an accuracy of ~ ± 0.2% relative, which may be necessary to establish resolution and elution order of the closest resolvable pairs. This problem is particularly acute when congeners not usually present in the technical mixtures appear and must be measured. All 209 congeners are now available from commerical distributors of standards, but it is still an expensive and time-consuming process to obtain them and to check a variety of HRGC columns to find the optimal one(s) for particular CQCS analysis requirements.

To aid in this process, the author assembled and organized a consortium of laboratories (cf. Table 1A and Acknowledgements) to acquire complete retention information on all 209 congeners on 27 HRGC systems comprising 20 distinct stationary phases. Additionally, the amounts of detectable congeners in 6 Aroclor mixtures were measured on 18 of these systems against the individual standards to provide semiquantiative congener distributions [2]. The purpose of this paper is to present an abbreviated retention database for 17 of the stationary phases *(plus one additional octyl system)* and discuss its usefulness in designing CQCS PCB analyses.

Experimental

Individual stock standard solutions of all 209 PCB congeners in 1.0 ml ampoules at 100 µg/ml in isooctane were purchased from AccuStandard Inc. (New Haven, CT, USA). The synthesis, purity, and spectroscopic and chromatographic properties of the congeners have been documented [15]. Six ampoules each containing one of Aroclors 1221, 1016, 1242, 1254, 1260, and 1262 at 1000 µg/ml in isooctane, and crystalline decachlorobiphenyl internal standard (I.S.) were purchased from the same source. Internal standard 2-fluorobiphenyl (2F-BP) was purchased from Aldrich Chemical Company, (Milwaukee, WL, USA). Using PCB retention data from SE-54 [13], SB-octyl-50 [17, 18], and DB-1 [3] capillary columns as a guide, the 209 congeners were divided among 30 isooctane solutions by precisely pipetting 7 of the stock congener solutions plus stock solutions of both internal standards to 25 ml volumetric flasks to produce mixtures of 9 components each at 4 µg/ml, designed to elute at broad, evenly-spaced intervals. The 6 Aroclor solutions were likewise prepared at 40 µg/ml, with the 2 internal standards at 4 µg/ml, as well as blank isooctane solvent with the 2 internal standards. Consortium labs employing MS-SIM detection received 1.0 ml aliquots of the 37 solutions in amber, Hewlett-Packard autosampler vials capped with red-top, teflon-lined, crimp-top seals. Because of the superior absolute sensitivity and more limited dynamic range of ECDs, labs employing these detectors received solutions sets diluted 12.5-fold to 0.32 µg/ml of congeners and internal standards and 3.2 µg/ml of Aroclors.

Mixture 3 contained PCBs 52 and 180, and it was reinjected after every 6th sample in the injection sequence of 37 samples. Following Ballschmiter [17, 18], relative retention times (RRTs) for all peaks were calculated against the sum of the retention times (RTs) of PCBs 52 and 180, and the values were adjusted by interpolation for any observed consistent drift observed from the repeated injections of Mix 3. These 2 external RRT standards eluted in the middle of the first and last halves of the range of congener elutions, and their separate injection avoided any coelution with other congeners on the wide variety of columns tested. They were superior for this purpose to the internal relative response factor (RRF) standards, which eluted at either extreme of the range. Individual congener ECD RRFs were calculated against the PCB 209 (decachlorobiphenyl) I.S., while MS-SIM RRFs were calculated against both I.S.'s, and the I.S. providing the most stable ratios was used for subsequent calculations. To assess system resolution, analysts were requested to measure the peak widths at half height (W@1/2H) of the two RRT external standard congeners.

Elution data were acquired for the 27 systems described in Table 1A. Analysts in the consortium were instructed to optimize linear flow velocity and temperature programs to ensure elution of all congeners during the slow temperature ramp. System temperature programs and carrier gas flow parameters are displayed in Table 1B. System 3 employed full-scan, ion-trap, mass-spectrometric detection using a Varian Saturn ion-trap GC-MS; all other GC-MS systems employed a uniform SIM acquisition on Hewlett-Packard 5971 or 5972 bench-top instruments. Analysts were instructed to acquire SIM data in 5 groups of 4 masses, each with dwell times resulting in 5 acquisition cycles per second. The 4 masses in the groups, and the group acquisition times were adjusted to ensure measurement of all congeners eluting within the windows at either their M^+, M^++2, or M^++4 masses; namely, 172.0, 188.0, 221.9, 255.9, 291.9, 325.8, 359.8, 395.8, 429.7, 463.7, and 497.7 atomic mass units for 2F-BP internal standard, and chlorobiphenyls with 1 to 10 chlorines, respectively. Members of the consortium submitted peak RTs and areas obtained from their instruments' data systems for the I.S.'s, 208 congeners in the 30 mixes [congener 209 was used as I.S.], and the 6 Aroclors, via Excel 4.0 (Microsoft Inc., Redmond, WA, USA) spreadsheets to the author, who reduced, checked and edited the information for incorporation into the database.

Results

The procedures for and results of the determination of congener distributions in the 6 Aroclors are reported in the 2nd paper of this study [2]. To save space, 18 of the 27 systems listed in Tables 1A and 1B were selected for display of an abbreviated retention database in Table 2. Systems 2, 3, 5, 7, 9, and 23 were omitted since their stationary phase was represented in another system. Systems 18 and 19 were omitted since unusually large peak widths led to prediction of excessive numbers of congener coelutions. System 25 employed an experimental phase not commercially available, while that of 26 may be marketed by J&W Scientific. Two SB-octyl systems (4 and 6) were chosen from four available to illustrate the greatest variability among systems of the same phase. The complete retention database for all 27 systems in both the format of Table 2 and also listed in order of IUPAC congener number is available as supplementary material (see below).

The response factors relative to the I.S.'s for each congener in each system (RRFs) were compiled and are available in the supplementary material. These varied substantially among the instruments employed in the different systems. The mean value (for all congeners in the homolog group(s)) of the percent relative standard deviations of the means of RRF values for 11 ECD systems, for the least sensitive mono- and dichlorobiphenyls was ± 63%, and this degree of variation decreased smoothly with increasing chlorination to a value of ±18% for octa- and nona-chlorobiphenyls. For 6 MS-SIM systems the corresponding values for RRFs vs 2F-BP followed the opposite trend, ranging from ± 12% to ± 42%, as expected from the opposite relation of MS-SIM response to chlorine number. While the RRFs for individual systems were useful

Table 1A Capillary GC systems characteristics, researchers, references from other work, and Aroclor PCB coelutions

	Sys No.	☐	Column	Silicone Substitution	Len. (m)	I. D. (mm	Film (u)	Analyst	Company	Det.	W@ 1/2H	# of Coel.	No. of #	# of < >	# of ACE	# of NCE	Ref #s	209I (min)
*	1	☐	DB1	100% A	30	.25	.25	G. Frame	GE	ECD	.060	55	35	20	2	3	11	40
	2	☐	DB1	100% A	30	.25	.25	G.Frame	GE	MS	.064	55	38	17	1	4	"	49
	3	☐	RTX-1	100% A	60	.25	.25	J. Cochrane	HWRIC	MS-IT	.084	45	31	14	1	1	"	87
*	4	☐	SPB-Octyl	100% E	30	.25	.25	G. Frame	GE	ECD	.053	47	23	24	0	2	17,18	45
	5	☐	SPB-Octyl	100% E	30	.25	.25	G. Frame	GE	ECD	.053	41	17	24	1	1	"	50
*	6	☐	SPB-Octyl	100% E	60	.25	.25	J. Cochrane	HWRIC	ECD	.135	36	25	11	1	1	"	104
	7	☐	SPB-Octyl	100% E	30	.25	.25	N. Erwin	Supelco	MS	.077	51	29	22	1	1	"	58
*	8	☐	CP-Sil5-C18	100% D	100	.25	.10	E. deWitte	Chrompack	ECD	.200	50	39	11	6	3	16,19	165
	9		CP-Sil5-C18	100% D	100	.32	.10	D. L. Poster	NIST	ECD	.195	35	18	17	5	3	"	156
*	10		DB5-MS	5% K	30	.25	.50	M. Hastings	J&W	MS	.085	52	35	17	4	8		73
*	11	☐	RTX-5	5% B	60	.25	.25	C. Loope	Restek	MS	.118	60	35	25	4	4	11,13,16	106
*	12	☐	CP-Sil 13	14% B	50	.25	.20	E. deWitte	Chrompack	ECD	.100	39	22	17	3	5	9	84
*	13	☐	SPB-20	20% B	30	.25	.25	N. Erwin	Supelco	MS	.070	55	30	25	3	5		57
*	14		HP-35	35% B&C	30	.25	.25	I. Chang	H-P	MS	.053	63	41	22	9	6		35
*	15	☐	RTX-35	35% B	60	.25	.25	C. Loope	Restek	MS	.121	52	33	19	5	3		119
*	16		DB-17	50% B	30	.25	.25	M. Hastings	J&W	MS	.066	64	47	17	15	6	9,15	51
*	17	☐	HP-1301	6% G	60	.25	.25	I. Chang	H-P	MS	.051	55	25	30	4	8		41
	18		AT-1701	14% G	30	.25	.25	S. Miller	Alltech	MS	.065	68	42	26	19	11	11	42
	19		007-ODP	80%D;15%B	50	.25	.10	J.Criscio	Quadrex	ECD	NA						15	118
*	20	☐	DB-XLB	Proprietary	30	.25	.50	M. Hastings	J&W	MS	.065	34	12	22	3	6		77
*	21		DB35-MS	35%B&C+	30	.25	.25	M. Hastings	J&W	MS	.064	56	30	26	9	6		77
*	22	☐	HT-8	X%L; Y%B	50	.22	.25	M. Cumbers	SGE	ECD	.090	60	28	32	5	7	12	57
	23	☐	CNBP#1	XX%J	25	.25	.25	B. Hillery	NIST	ECD	.125	59	27	32	9	7	20	76
*	24	☐	Apiezon L	Hydrocarbon	30	.25	.25	E. Barnard	NYSDOH	ECD	.110	64	51	13	7	7	21,22	61
	25		Polyimide	Polyimide	30	.25	.25	S. Miller	Alltech	ECD	.065	54	28	26	8	8		51
*	26		CNBP#2	XX%J	30	.32	.25	M. Hastings	J&W	MS	.090	53	24	29	6	7	20	76
*	27		007-23	78% H	48	.25	.10	G. Frame	GE	MS	.098	58	30	28	23	7	9	60

* Indicates system listed in Table 2 (Congener Elution Order)

No. of # indicates number of coeluting PCB isomers or congeners coeluting with +2Cl homologs, found in Aroclors
\# of < > indicates number of coeluting homologs in Aroclors differing by 1 Cl, potentially resolvable by MS detection
\# of Coel. is sum of above 2 categories, the number of coeluting congeners in Aroclors not resolvable with ECD
Ref #s are references in the bibliography of papers containing retention data for many congeners on similar phases
\# of ACE is number of "close elutions" (<6 W@1/2H units) in calibration mixes 1,2,3,4 & 5 (144 Aroclor PCBs)
\# of NCE is number of "close elutions" (<6 W@1/2H units) in calibration mixes 6, 7, 8 & 9 (65 non- Aroclor PCBs)
NA indicates peak width not measured, therefore coelutions not predictable

W@1/2H is mean of peak widths at half height of PCBs 52 and 180 in system.

209IS is the retention time in minutes of the PCB #209 internal standard, the last peak to elute, indicative of analysis time

Companies are GC column manufacturer's labs except for the following abbreviations:

GE = General Electric Corporate R&D; HWRIC = Illinois Hazardous Waste Research & Information Center
NIST = Natl. Inst. of Standards & Technology; NYSDOH = New York State Dept. of Health, Wadsworth Lab

☐ = System included in minimum No. of Calibrating Mixes Calculation

Key to Polydimethylsiloxane-based Stationary Phase Structures

A	Me-Si-Me	P = phenyl
B	P-Si-P	Me = methyl
C	P-Si-Me	C8 = n-octyl
D	C18-Si-Me	C18 = n-octadecyl
E	C8-Si-Me	CyP = 3-cyano, n-propyl
G	CyP-Si-P	CyBA = p-cyano, p'-allyloxy biphenyl
H	CyP-Si-CyP	C = m-carborane
J	CyBA-Si-Me	
K	O-Si-P-Si-O	
L	O-Si-C-Si-O	

for quantifying Aroclor congeners with them, the extent of variation serves to emphasize the danger of quantitative error in using published values instead of acquiring them against suitable standards on the analyst's own system. Therefore the RRF database is not presented here.

Table 2 displays the elution order of all 209 congeners on the 18 systems starred in Tables 1A and 1B. These are

Table 1B GC column injection, column pressure and temperature parameters

	Sys. No.	Column	Col. Len. (m)	Det.	Head Press. psig	Flow cm/ sec	Flow Temp. C	Init. Temp C	Init Hold min	1st Rate C/min	1st Break C	2nd Rate C/min	Final Temp C	Inj Temp C	Inj Mode 1 ul	Det. Temp C
					Carrier Gas Data			Column Temperature Program Values						Injector Port		
*	☐ 1	DB1	30	ECD	35.2	47.8	210	90	2	15	165	2.5	255	270	Sless	300
	☐ 2	DB1	30	MS	14.8	39.6	150	75	2	15	150	2.5	260	270	Sless	280
	☐ 3	RTX-1	60	MS-IT	30.0	25.1	218	75	2	15	150	1.5	285	250	Sless	250
*	☐ 4	SPB-Octyl	30	ECD	24.0	35.9	223	90	2	15	165	3	280	270	Sless	300
	☐ 5	SPB-Octyl	30	ECD	24.0	37.5	193	75	2	15	150	3	270	300	Sless	300
*	☐ 6	SPB-Octyl	60	ECD	35.0	55.2	210	75	2	15	150	1.2	270	250	Sless	295
	☐ 7	SPB-Octyl	30	MS	10.3	37.5	215	75	2	15	150	2.5	280	270	Sless	290
*	☐ 8	CP-Sil5-C18	100	ECD	50.1	22.3	209	75	2	15	150	0.75	268	275	Sless	300
	9	CP-Sil5-C18	100	ECD	36.7	28.2	200	75	2	15	150	0.75	250	250	SPLIT	300
*	10	DB5-MS	30	MS	17.0	33.2	150	100	1			2.5	285	250	OnCol	320
*	☐ 11	RTX-5	60	MS	26.5	21.2	300	75	2	15	150	1.2	300	250	Sless	310
*	☐ 12	CP-Sil 13	50	ECD	32.9	30.5	208	75	2	15	150	1.5	266		Sless	300
*	☐ 13	SPB-20	30	MS	9.1	33.6	215	75	2	15	150	2.5	280	270	Sless	290
*	14	HP-35	30	MS	9.4	33.7	280	80	1	25	180	3	280	260	Sless	300
*	☐ 15	RTX-35	60	MS	28.0	24.1	300	75	2	15	150	1.2	300	250	Sless	310
*	16	DB-17	30	MS	17.0	33.1	195	100	1			3	290	250	OnCol	300
*	☐ 17	HP-1301	60	MS	39.0	30.0	300	80	1	25	180	3	300	270	Sless	300
	18	AT-1701	30	MS	1.0	18.0	250	90	2	15	165	3	330	300	Sless	300
	19	007-ODP	50	ECD	11.0	10.6	200	75	2	15	150	1.5	250	230	Sless	300
*	☐ 20	DB-XLB	30	MS		33.3	150	100	1			2.5	293	250	OnCol	340
*	21	DB35-MS	30	MS		33.3	150	80	1			2.5	285	250	OnCol	320
*	☐ 22	HT-8	50	ECD	40.0	29.8	320	80	2	30	170	3	320	300	SPLIT	330
	☐ 23	CNBP#1	25	ECD	23.0	42.1	211	75	5	4	155	2	250	270	SPLIT	300
*	☐ 24	Apiezon L	30	ECD	30.0	45.3	205	100	2	10	160	2	250	250	Sless	300
	25	Polyimide	30	ECD	17.0	24.4	263	150	2	15	225	2	300	300	Sless	325
*	26	CNBP#2	30	MS		33.5	150	80	1			2.5	270	250	OnCol	290
*	27	007-23	48	MS	11.0	20.2	190	75	2	15	150	1.5	230	270	Sless	280

Notes:

Retention time of PCB 209 in System 19 indicates linear flow greatly exceeded Van Deempter optimum
Resolution was degraded, but Aroclor quantities of resolved peaks were in good agreement with averages.
Reported pressure parameters not consistent with elution times.

Helium was carrier gas for all systems, except for hydrogen in System 6

Systems 2, 14 and 17 used electronic pressure control in constant flow mode at start of slow temperature ramp.

Linear flow velocity at indicated temperature either measured by timing elution of methylene chloride vapor injection or calculated using Hewlett-Packard PC flow calculator from column dimensions and pneumatic parameters.

☐ = System included in minimum No. of Calibrating Mixes Calculation

* Indicates system listed in Table 2 (Congener Elution Order)

Injection Modes: SPLIT; Sless = Splitless; OnCol = Hot (250 C.) on column to 1m x 0.53 mm fused silica retention gap installed ahead of analytical column

Linear flow velocities and temperature programs were adjusted to ensure all congeners eluted during the slow temperature ramp. System 26 data chosen to illustrate CNBP phase since system 23 used a 10 min hold at 211 C to improve critical congener resolution.

listed as pairs of IUPAC congener numbers and relative retention times. *The numbers for congeners 107, 108, 109, 199, 200 and 201 in this paper are derived according to Guitart et al. [27], and they differ from the corresponding numbers assigned by Ballschmiter and Zell [28] as 108, 109, 107, 201, 199 and 200, respectively.* See the 2nd paper [2] for assignment of chlorine substitution patterns to the congener numbers. IUPAC numbers of congeners reported in that paper to be present in any of Aroclors 1242, 1254 or 1260 above 0.05 weight% are displayed in Table 2 in **bold face**, and those above 1.0 weight% with **bold underline**.

The peak widths at half height (W@½H) of PCBs 52 and 180 were used to estimate W@½H for all other congeners by linear interpolation and extrapolation vs RT from the values of that pair. Studies of the Aroclor chromatograms from systems 1, 2, 4, 8 and 12 indicated that peaks could just be resolved and individually quantitated by instrument data systems if they eluted at or greater than one W@½H unit apart (with the exception of minor peaks

Table 2 Congener elution orders (PCB IUPAC # and relative retention time vs (52 + 180))

M #		System 1 100% C1		System 4 50% C8		System 6 50% C8		System 8 50% C18		System 10 DB5MS		System 11 5%Ph		System 12 13%Ph		System 13 20%Ph		System 14 35%Ph
1		1 .1704		1 .1719		1 .1214		1 .1261		1 .2301		1 .1534		1 .1504		1 .1870		1 .1724
1		2 .1876		2 .1804		2 .1482		2 .1554		2 .2654		2 .1772		2 .1725		2 .2104		2 .1890
1		3 .1897		3 .2005		3 .1507		3 .1579		3 .2692		3 .1800		3 .1757		3 .2139		3 .1918
1	#	4 .2006		4 .2039		4 .1543		4 .1608	#	4 .2856	#	4 .1957	#	10 .1929		10 .2326		10 .2066
2	#	10 .2008		10 .2059		10 .1567		10 .1630	#	10 .2857	#	10 .1958	#	4 .1936		4 .2337		4 .2079
1	#	9 .2160		9 .2284		9 .1824		9 .1882	#	7 .3095	#	9 .2149	#	7 .2098	#	7 .2483	#	7 .2173
2	#	7 .2164		7 .2304		7 .1850		7 .1904	#	9 .3099	#	7 .2154	#	9 .2099	#	9 .2487	#	9 .2181
1		6 .2221		6 .2346		6 .1883		6 .1941		6 .3186		6 .2238		6 .2201		6 .2593		6 .2265
1	#	8 .2257		5 .2388		5 .1930		5 .1987		5 .3237		8 .2289		8 .2256		8 .2647		8 .2315
2	#	5 .2262		8 .2402		8 .1947		8 .2005		8 .3246		5 .2301		5 .2271		5 .2669		5 .2339
4		14 .2368		19 .2450		19 .1993		19 .2050		14 .3373		14 .2412		14 .2333		14 .2703		14 .2351
1		19 .2382		14 .2603		14 .2195		14 .2252		19 .3402		19 .2473		19 .2467		30 .2835		30 .2466
8		30 .2477		30 .2659		30 .2273		30 .2305		30 .3477		30 .2550		30 .2468		19 .2868		19 .2534
6		11 .2493		18 .2686		18 .2277		18 .2324		11 .3552		11 .2593		11 .2539		11 .2908		11 .2548
4	#	13 .2529		11 .2732		11 .2322		17 .2380		12 .3592	#	12 .2645		12 .2600		12 .2969	#	12 .2610
5	#	12 .2535		17 .2737		17 .2340		11 .2383	>	13 .3607	#	13 .2648		13 .2613		13 .2981	#	13 .2617
1	<	18 .2561	<	27 .2774	#	13 .2365		27 .2418	<	18 .3610		18 .2678		18 .2648	#	18 .3020	#	18 .2649
3	>	15 .2565	#	13 .2777	#	12 .2373	#	13 .2434		17 .3626	<	17 .2696		17 .2659	#	17 .3028	#	17 .2651
2		17 .2576	#	12 .2780	<	27 .2373	#	12 .2436		15 .3660	>	15 .2701		15 .2672		15 .3036		15 .2669
3	#	27 .2638		24 .2790		24 .2394	<	24 .2440	#	27 .3694	#	27 .2780	#	27 .2750	#	27 .3114		27 .2737
2	#	24 .2642		16 .2818	<	16 .2409		16 .2455	#	24 .3696	#	24 .2781	#	24 .2752	#	24 .3119		24 .2755
1	#	16 .2694		15 .2824	>	15 .2416		15 .2488		16 .3763	#	32 .2860		32 .2841		32 .3183		34 .2806
2	#	32 .2705		54 .2870		54 .2464		54 .2507		32 .3777	#	16 .2863		16 .2859	#	34 .3219		32 .2824
4		54 .2796		32 .2875		32 .2491		32 .2526		34 .3852		34 .2947		34 .2884	#	16 .3227		23 .2830
3		34 .2801		34 .3030		34 .2694		34 .2726		23 .3855		23 .2955		23 .2891		23 .3228	#	29 .2860
9		23 .2807		23 .3048		23 .2717		23 .2750		54 .3879		29 .2990		29 .2923		29 .3257	#	16 .2862
3		29 .2839	#	29 .3092	#	26 .2764	#	29 .2802		29 .3887		54 .2995		26 .2992		26 .3321		26 .2930
2		26 .2868	#	26 .3101	#	29 .2771	#	26 .2805		26 .3950		26 .3040		25 .3020		25 .3346		25 .2945
1		25 .2886		25 .3132	>	25 .2802		25 .2843		25 .3960		25 .3065		54 .3020		54 .3387		50 .3010
2		31 .2933		50 .3132	<	53 .2810		31 .2902		50 .3987		31 .3122		50 .3072		50 .3402	#	28 .3020
1		28 .2945		53 .3149		50 .2815	#	28 .2941	#	31 .4024		50 .3124		31 .3087		31 .3410	#	31 .3024
6		50 .2947		31 .3177		31 .2855		50 .2942	#	28 .4028		28 .3137		28 .3098		28 .3420		54 .3047
6		21 .3018		28 .3218	#	28 .2902	#	20 .2949		21 .4078		21 .3228		21 .3205		21 .3529		33 .3147
3	#	20 .3022		20 .3236	#	20 .2906	#	53 .2949	<	53 .4091	#	33 .3235		33 .3214		33 .3531		21 .3151
5	#	33 .3026	#	51 .3246		45 .2915	#	51 .2950	#	20 .4092	#	20 .3237	>	20 .3225		20 .3545		20 .3174
4	<	53 .3033	#	45 .3249		51 .2928	#	45 .2954	#	33 .4093	<	53 .3244	<	53 .3234		53 .3555		36 .3190
4	<	51 .3079		21 .3251		21 .2928		21 .2969		51 .4133		51 .3293		51 .3281		36 .3581		53 .3191
1	>	22 .3081		33 .3261		33 .2940		33 .2978		22 .4159		22 .3310		36 .3299		51 .3597		51 .3226
2		45 .3136		46 .3301		46 .2968		46 .3003		45 .4188		45 .3365		22 .3315		22 .3630		22 .3259
7		36 .3172		22 .3321		22 .3001		22 .3044		36 .4225		36 .3372		45 .3374		69 .3680		69 .3288
2		46 .3204		52 .3472		52 .3206		52 .3246		46 .4251		46 .3451		69 .3407		45 .3689		39 .3316
9		39 .3237		73 .3485		73 .3230		73 .3248		69 .4276		39 .3464		39 .3418		39 .3694		73 .3320
1		52 .3280		43 .3504		43 .3244		43 .3265		73 .4288		69 .3483		73 .3447		73 .3717		45 .3350
3		69 .3281		69 .3517		36 .3265		69 .3293		39 .4297		52 .3499		52 .3463		52 .3739		52 .3377
4		73 .3296		36 .3520		69 .3279		49 .3308	#	43 .4317		73 .3508		46 .3475	#	43 .3773	#	43 .3398
8	#	43 .3317		49 .3539		49 .3286		36 .3315	#	52 .4317		43 .3536		43 .3498	#	49 .3777	#	49 .3403
5	#	49 .3321		39 .3575		39 .3323		48 .3345		49 .4345		49 .3547		49 .3510	#	46 .3783	#	75 .3405
6		38 .3346		48 .3580		48 .3332		104 .3352		38 .4356		38 .3565		38 .3515		38 .3786	#	47 .3414
3		47 .3348		104 .3603		104 .3362	#	47 .3385	#	48 .4362	#	47 .3571		75 .3525	#	75 .3788		38 .3425
2	#	48 .3367		65 .3609		44 .3366		39 .3386	#	47 .4366	#	75 .3578		47 .3535		47 .3799	#	48 .3443
4	#	75 .3367		47 .3610		65 .3372	#	44 .3389	#	75 .4367	#	48 .3586		48 .3546		48 .3814	#	46 .3450
6		65 .3400		44 .3627		47 .3377		65 .3391		65 .4374		65 .3618		65 .3565		65 .3832		65 .3487
9		62 .3419		62 .3646		38 .3417		62 .3429		62 .4384		62 .3627		62 .3576		62 .3837		62 .3489
4		35 .3425		75 .3647		62 .3418		75 .3436		104 .4424		104 .3668		104 .3648		35 .3909		104 .3561
5		104 .3447		38 .3664		96 .3420		59 .3446		35 .4457		35 .3669		35 .3654		104 .3912		35 .3573
1		44 .3467		59 .3671		59 .3421		96 .3446		44 .4471		44 .3718	#	44 .3721		72 .3959		72 .3586
2	>	37 .3489		96 .3685		75 .3432		38 .3466		59 .4484		59 .3743	#	59 .3728	#	59 .3978		68 .3646
5	#	59 .3500		42 .3700		42 .3454		42 .3469		42 .4495	>	37 .3753		72 .3740	#	44 .3979	#	59 .3652
3	#	42 .3502		35 .3746		35 .3494	#	41 .3538		37 .4521	<	42 .3755	>	37 .3756	>	37 .4003	#	44 .3655
1	#	71 .3592	#	41 .3761		41 .3517	>	35 .3547	#	71 .4555		72 .3812	<	42 .3758	<	42 .4009		42 .3671
2	#	41 .3592	#	71 .3770	#	40 .3535	#	71 .3554		72 .4563		71 .3836		68 .3806		68 .4017		37 .3684
5	#	64 .3593		40 .3788	#	71 .3541	#	40 .3562	#	41 .4566	#	41 .3851		71 .3835		71 .4075		71 .3748
7		72 .3601	<	64 .3800		37 .3561		64 .3596		64 .4575	#	64 .3852	#	64 .3858		103 .4097		103 .3759
7		96 .3638	>	37 .3809		64 .3575		37 .3623		68 .4587		68 .3863	#	41 .3864		64 .4098		57 .3785
9		68 .3642		72 .3893		72 .3721		72 .3745		96 .4602		96 .3902		103 .3887		41 .4107	#	64 .3790
3		40 .3663		103 .3917		103 .3749		103 .3750		40 .4625		40 .3938		57 .3908		57 .4114	#	41 .3798
6		57 .3733		68 .3935		94 .3770		94 .3794		103 .4633		103 .3941		96 .3938		100 .4151		100 .3811
2		103 .3736		94 .3970		68 .3770		68 .3799		57 .4656		57 .3952		100 .3952		67 .4158		67 .3835
1		67 .3783		57 .4004		57 .3838		95 .3875		100 .4680		100 .4000		67 .3960		96 .4181		58 .3889
4		100 .3792		100 .4037		95 .3861		100 .3877		67 .4693		67 .4005		40 .3980		58 .4210		80 .3905
8		58 .3801		95 .4046		58 .3881		58 .3906		58 .4709		58 .4038		58 .4014		40 .4216		96 .3914

Table 2 (continued)

System 15 35%Ph		System 16 50%Ph		System 17 6%CyPP		System 20 DB-XLB		System 21 DB35MS		System 22 8%PhCS		System 24 Apiezon L		System 26 CNBP#2		System 27 78%CyP	
1	.1682	1	.2207	1	.1989	1	.2324	1	.2259	1	.1858	1	.1246	1	.2255	1	.1838
2	.1916	2	.2453	2	.2196	2	.2704	2	.2565	2	.2161	4	.1508	2	.2714	2	.2138
3	.1963	3	.2498	3	.2225	3	.2776	3	.2627	3	.2191	2	.1527	10	.2719	10	.2149
10	.2191	10	.2774	10	.2341	4	.2864	10	.2790	10	.2285	10	.1534	4	.2745	3	.2200
4	.2213	4	.2802	4	.2351	10	.2871	4	.2806	4	.2304	3	.1551	3	.2801	7	.2213
# 7	.2326	7	.2873	# 9	.2487	9	.3127	7	.2964	9	.2497	9	.1802	9	.2969	4	.2225
# 9	.2329	9	.2885	# 7	.2490	7	.3138	9	.2970	7	.2519	# 7	.1832	7	.2997	9	.2241
6	.2463	6	.3016	6	.2581	6	.3205	6	.3069	6	.2635	# 6	.1844	6	.3089	30	.2331
8	.2522	14	.3037	8	.2623	5	.3262	8	.3135	# 8	.2679	> 5	.1876	# 5	.3162	6	.2417
14	.2533	8	.3071	5	.2635	8	.3284	5	.3144	# 5	.2687	< 19	.1881	# 8	.3166	8	.2484
5	.2564	5	.3122	14	.2708	19	.3401	14	.3185	19	.2795	8	.1916	19	.3220	14	.2504
30	.2694	30	.3212	19	.2783	14	.3431	30	.3285	14	.2815	18	.2172	30	.3253	5	.2519
11	.2786	11	.3283	30	.2790	30	.3508	19	.3329	30	.2858	30	.2192	14	.3351	# 19	.2691
19	.2813	# 12	.3355	11	.2886	11	.3612	11	.3396	18	.3006	14	.2201	18	.3407	# 17	.2693
12	.2855	# 13	.3361	< 18	.2936	18	.3615	12	.3450	11	.3024	# 17	.2246	17	.3430	18	.2733
# 18	.2939	< 19	.3367	# 12	.2937	17	.3637	18	.3463	17	.3039	# 27	.2252	# 27	.3499	23	.2781
> 13	.2941	15	.3422	# 13	.2940	12	.3655	17	.3468	# 13	.3082	# 16	.2274	# 24	.3504	34	.2798
# 17	.2943	# 17	.3439	17	.2948	< 27	.3691	13	.3479	< 24	.3092	54	.2278	11	.3568	# 29	.2817
> 15	.2946	# 18	.3441	15	.2993	> 13	.3694	27	.3539	# 12	.3092	# 24	.2284	32	.3572	# 24	.2823
27	.3042	27	.3531	24	.3022	24	.3716	15	.3551	27	.3122	11	.2322	16	.3599	27	.2856
24	.3052	# 34	.3543	27	.3030	16	.3761	24	.3557	15	.3146	12	.2365	54	.3603	50	.2866
34	.3100	# 24	.3544	32	.3094	15	.3780	# 34	.3624	32	.3191	> 13	.2382	12	.3643	32	.2940
23	.3122	23	.3568	16	.3117	32	.3791	# 32	.3630	16	.3221	< 32	.2387	> 13	.3662	11	.2947
32	.3141	29	.3596	23	.3144	54	.3861	23	.3642	54	.3263	15	.2450	< 34	.3668	12	.2998
29	.3150	32	.3617	34	.3149	34	.3865	16	.3647	23	.3288	34	.2624	23	.3673	25	.3032
16	.3196	26	.3658	29	.3173	23	.3880	29	.3669	34	.3306	53	.2639	50	.3682	13	.3051
26	.3221	# 16	.3681	54	.3228	29	.3909	26	.3742	29	.3331	23	.2645	29	.3714	26	.3070
25	.3251	# 25	.3681	26	.3237	26	.3973	25	.3759	26	.3390	50	.2668	15	.3754	16	.3101
# 31	.3324	# 31	.3745	25	.3257	50	.3979	50	.3774	50	.3390	# 26	.2710	26	.3780	28	.3137
< 50	.3330	# 28	.3752	50	.3286	25	.3996	54	.3784	25	.3426	# 29	.2710	53	.3806	54	.3142
# 28	.3333	50	.3763	31	.3307	31	.4065	31	.3828	31	.3459	45	.2734	25	.3816	69	.3154
54	.3398	36	.3818	28	.3319	53	.4071	28	.3835	< 53	.3493	> 25	.2759	51	.3835	< 31	.3169
36	.3462	54	.3870	21	.3410	28	.4086	> 33	.3903	> 28	.3497	# 46	.2766	31	.3863	> 15	.3175
33	.3475	33	.3880	< 53	.3421	# 33	.4105	21	.3906	51	.3549	# 51	.2774	28	.3902	51	.3210
21	.3491	21	.3893	> 33	.3424	21	.4108	< 53	.3909	21	.3578	# 31	.2817	45	.3925	53	.3237
20	.3500	20	.3906	20	.3434	# 20	.4109	20	.3920	# 20	.3607	# 20	.2823	21	.3949	73	.3242
53	.3522	53	.3936	51	.3455	51	.4120	51	.3945	# 33	.3609	21	.2844	33	.3956	104	.3246
51	.3561	39	.3938	22	.3500	45	.4181	36	.3966	< 45	.3613	33	.2858	20	.3965	75	.3268
69	.3588	69	.3951	36	.3531	22	.4198	22	.4005	22	.3674	28	.2875	104	.3991	21	.3299
39	.3599	51	.3966	45	.3538	46	.4232	69	.4007	46	.3716	22	.2939	46	.3992	62	.3338
22	.3599	22	.3987	69	.3584	73	.4269	73	.4012	36	.3730	73	.3095	73	.4003	< 47	.3341
73	.3643	73	.3989	39	.3614	36	.4287	45	.4031	69	.3743	# 52	.3099	69	.4012	> 33	.3351
52	.3670	52	.4027	# 52	.3625	69	.4296	# 43	.4072	52	.3744	# 43	.3102	# 43	.4037	# 49	.3379
45	.3688	38	.4045	# 46	.3626	43	.4304	# 52	.4072	73	.3762	104	.3161	# 52	.4038	65	.3379
# 75	.3721	75	.4051	73	.3626	52	.4313	39	.4074	# 43	.3783	69	.3180	22	.4051	# 48	.3388
38	.3726	49	.4059	# 43	.3652	48	.4338	# 49	.4099	# 49	.3790	96	.3188	49	.4069	155	.3390
# 49	.3728	# 43	.4067	# 49	.3656	49	.4354	# 46	.4099	39	.3808	# 49	.3192	48	.4079	< 52	.3425
# 43	.3728	# 47	.4074	75	.3666	39	.4380	# 48	.4108	104	.3822	# 48	.3194	75	.4090	> 20	.3436
47	.3746	# 45	.4079	47	.3678	104	.4383	# 75	.4110	# 75	.3831	44	.3228	47	.4101	45	.3469
48	.3772	48	.4106	48	.3694	47	.4383	# 47	.4115	65	.3834	65	.3249	65	.4119	100	.3469
65	.3788	65	.4113	65	.3709	65	.4390	38	.4122	# 47	.3841	# 59	.3296	62	.4121	103	.3486
62	.3798	62	.4120	38	.3711	62	.4396	65	.4134	# 48	.3841	62	.3298	36	.4173	36	.3524
46	.3805	72	.4128	62	.3718	75	.4398	62	.4138	62	.3862	36	.3300	96	.4219	68	.3557
72	.3854	35	.4161	104	.3752	38	.4402	104	.4178	38	.3929	# 47	.3300	44	.4220	22	.3558
35	.3863	46	.4178	> 35	.3834	44	.4461	35	.4244	44	.3968	42	.3333	59	.4245	72	.3606
104	.3899	68	.4190	< 44	.3841	# 59	.4487	72	.4249	59	.3985	# 75	.3361	103	.4246	121	.3617
68	.3925	104	.4224	59	.3858	# 42	.4493	# 44	.4258	42	.4014	# 40	.3368	42	.4256	43	.3619
59	.3953	> 37	.4256	42	.3869	35	.4518	# 59	.4259	96	.4038	# 41	.3369	39	.4276	39	.3659
< 44	.3969	< 59	.4257	72	.3886	71	.4531	42	.4283	35	.4043	39	.3391	100	.4281	46	.3664
> 37	.3972	44	.4275	37	.3914	41	.4549	68	.4286	64	.4064	71	.3398	71	.4285	38	.3763
42	.4003	80	.4293	68	.3924	96	.4565	71	.4320	72	.4066	38	.3419	41	.4316	# 42	.3801
103	.4037	57	.4296	# 71	.3946	72	.4582	103	.4326	103	.4079	64	.3477	72	.4326	# 59	.3803
57	.4050	42	.4303	# 64	.3947	64	.4602	37	.4339	71	.4088	35	.3529	64	.4328	94	.3820
71	.4068	103	.4304	41	.3962	> 37	.4610	41	.4355	41	.4102	94	.3597	38	.4329	57	.3839
# 64	.4101	67	.4338	103	.3979	< 40	.4611	64	.4368	68	.4118	103	.3620	94	.4346	44	.3840
# 67	.4101	71	.4353	96	.4004	103	.4612	57	.4369	37	.4123	37	.3630	155	.4360	96	.3879
100	.4104	100	.4353	57	.4021	68	.4619	100	.4370	100	.4146	95	.3698	68	.4370	71	.3885
80	.4113	64	.4372	100	.4023	100	.4667	67	.4404	40	.4193	72	.3715	102	.4401	< 102	.3899
41	.4121	121	.4378	# 67	.4065	57	.4677	96	.4412	57	.4201	93	.3725	40	.4412	> 67	.3903
58	.4166	58	.4392	# 40	.4066	94	.4688	58	.4430	94	.4216	102	.3751	98	.4428	98	.3909
121	.4188	41	.4405	58	.4110	67	.4717	94	.4443	67	.4254	68	.3775	57	.4444	61	.3930

Table 2 (continued)

M #	System 1 100% C1	System 4 50% C8	System 6 50% C8	System 8 50% C18	System 10 DB5MS	System 11 5%Ph	System 12 13%Ph	System 13 20%Ph	System 14 35%Ph
5	63 .3826	58 .4049	93 .3900 #	93 .3912	94 .4732	63 .4066	63 .4042	80 .4235	63 .3925
9	94 .3867	67 .4065	100 .3900 #	102 .3916	63 .4738	94 .4099	94 .4073	63 .4236	121 .3941
1	74 .3873	93 .4073	67 .3911	98 .3927	61 .4754	74 .4107	61 .4080	74 .4265	40 .3945
6	61 .3887	102 .4083	102 .3925	67 .3934	74 .4774	61 .4119	74 .4082	94 .4266	94 .3965
2	70 .3910	98 .4094	98 .3936	57 .3970	98 .4791	70 .4150	80 .4083	61 .4272	74 .3965
8	76 .3933	63 .4104	63 .3955	63 .3983	76 .4793	76 .4162	121 .4130	121 .4281	61 .3983
7	98 .3937	61 .4143	88 .3991	88 .3985	102 .4795	98 .4169 >	70 .4138	70 .4315	76 .4029
1	66 .3942	88 .4147	61 .3992	91 .4002	93 .4805	102 .4169	76 .4146	76 .4328	70 .4032
6	102 .3951 #	70 .4164 >	70 .4009	61 .4013	70 .4811	80 .4180	98 .4154	98 .4335 <	102 .4054
2	95 .3962 #	74 .4164 <	91 .4009	76 .4029 <	95 .4823 >	66 .4187 <	102 .4156	102 .4338	98 .4056
3	93 .3964 <	91 .4165	76 .4011	70 .4039 >	66 .4830	93 .4191	93 .4179	66 .4355 >	66 .4065
9	80 .3991	76 .4166	74 .4023	74 .4049	121 .4831 <	95 .4195	66 .4183	93 .4362	93 .4110
9	88 .4010 >	66 .4217	84 .4045	84 .4061	88 .4836	121 .4222	95 .4202	95 .4378	155 .4125
5	91 .4026 <	84 .4220	66 .4064	66 .4091	80 .4842	88 .4229	88 .4217	88 .4394	95 .4133
8	55 .4028	55 .4247	55 .4091	55 .4120	91 .4873	91 .4267	91 .4279	155 .4423	88 .4138
9	121 .4056	89 .4283	89 .4127	89 .4128	55 .4890	55 .4282	155 .4283	91 .4450	91 .4209
1 #	56 .4113	121 .4285	56 .4177	56 .4199	155 .4930	155 .4349	55 .4298	55 .4463	55 .4226
2 #	60 .4115	56 .4330	121 .4209	121 .4200 #	56 .4955 #	56 .4372	92 .4355	92 .4487	92 .4231
2	84 .4178 >	60 .4359	60 .4214	60 .4237 #	60 .4962 #	60 .4377 #	56 .4408	101 .4543	90 .4300
9	155 .4179 <	92 .4366	92 .4271	155 .4276	92 .4973	92 .4391 #	60 .4414	90 .4553	101 .4306
3	92 .4196	80 .4375	80 .4293	92 .4281	84 .4989	84 .4430 <	101 .4421 #	56 .4561 #	56 .4339
7	89 .4213	155 .4388	155 .4335	80 .4337	89 .5006 #	89 .4456	90 .4432 #	60 .4568 #	60 .4340
4	90 .4255	90 .4448	113 .4360	152 .4359	90 .5010 #	101 .4457	113 .4456	113 .4571	113 .4341
3	101 .4267	113 .4448	152 .4362	90 .4369	101 .5021	90 .4458 #	84 .4476	99 .4601	99 .4353
6	113 .4303	101 .4450	90 .4369	101 .4375	113 .5029	113 .4493 #	99 .4484	79 .4610	79 .4394
7	79 .4317	152 .4468	101 .4372 <	136 .4455	99 .5055	99 .4511	89 .4496	84 .4629	119 .4431
1	99 .4322	150 .4476	150 .4394 #	83 .4457	79 .5084	79 .4522	79 .4501	89 .4644 #	89 .4455
9	150 .4401 #	99 .4533 <	136 .4451 #	99 .4463	119 .5098	119 .4583	119 .4557	119 .4658 #	84 .4456
3	119 .4403 #	83 .4541 >	83 .4451	113 .4472	150 .5101	150 .4592	112 .4580	112 .4684	150 .4503
8	112 .4426	136 .4563	99 .4467	150 .4473	112 .5107	112 .4610	150 .4587	150 .4699	112 .4508
2	83 .4431	112 .4564	112 .4491	145 .4484	108 .5126	108 .4639	108 .4607	108 .4709	111 .4513
7	78 .4440	145 .4589	145 .4505	112 .4502	83 .5129	83 .4642	78 .4624	78 .4717	108 .4530
8	108 .4456	119 .4606	108 .4548 #	119 .4544	152 .5152	78 .4647	83 .4645	111 .4731	78 .4546
7	152 .4484	108 .4611	79 .4550	86 .4550	78 .5159	152 .4675	111 .4671	83 .4745	83 .4567
5	97 .4494	86 .4628	86 .4554	108 .4552	97 .5173	97 .4694	152 .4689	120 .4785	120 .4586
6	86 .4519	79 .4629 #	119 .4556 #	97 .4552	86 .5174	86 .4707	86 .4705	152 .4790	148 .4595
4	81 .4530	97 .4631 #	97 .4557	125 .4561	125 .5183	125 .4718	97 .4710	148 .4795	125 .4621
9	125 .4542	125 .4642	87 .4572	87 .4576	116 .5200	111 .4732	125 .4720	97 .4800	97 .4635
4 #	117 .4546	87 .4656	125 .4572	79 .4610	117 .5206 #	117 .4742	116 .4733	86 .4804	86 .4637
1 #	87 .4548	117 .4717	78 .4650 #	117 .4664	145 .5210	81 .4748	148 .4736	125 .4805	152 .4639
6	145 .4566	78 .4721	117 .4666 #	85 .4668	111 .5221	145 .4748	120 .4737	116 .4818	154 .4690
2	115 .4573	116 .4730	116 .4678	116 .4681 #	115 .5221 #	87 .4748	117 .4749 #	117 .4832 #	117 .4690
9	116 .4585	85 .4744	85 .4682	78 .4700 #	87 .5227 #	115 .4757	145 .4762 #	115 .4840 #	115 .4696
5	85 .4594 #	115 .4763	110 .4711 #	110 .4713	148 .5232	116 .4759 #	115 .4764	81 .4848	116 .4702
9	111 .4595 #	110 .4771	81 .4724 #	115 .4713	81 .5237	148 .4793	81 .4771	145 .4851	145 .4708
3	136 .4627	148 .4773	115 .4725	148 .4747	85 .5253	120 .4797	87 .4781	87 .4861	81 .4717
5	77 .4645	81 .4800	82 .4762	82 .4766	120 .5265	85 .4799	154 .4824	154 .4870	87 .4725
8	120 .4661	82 .4834	148 .4778	81 .4787	136 .5274	136 .4830	85 .4835	85 .4911	85 .4770
9	148 .4666	111 .4839	77 .4821	111 .4857	110 .5298 >	77 .4862	136 .4884 >	110 .4961 >	110 .4860
1	110 .4674 #	151 .4889	111 .4844 #	151 .4871	154 .5301 <	110 .4863 <	110 .4897 <	136 .4963 >	77 .4871
4	154 .4760 >	77 .4894	151 .4874 >	77 .4877	77 .5319	154 .4878 >	77 .4902	77 .4963 <	136 .4875
1	82 .4784	154 .4900	135 .4885 #	135 .4879	82 .5378	82 .4989	151 .4990	151 .5019	151 .4937
3	151 .4882 #	135 .4904	120 .4922	154 .4883	151 .5389	151 .5007	144 .5044 #	144 .5065	124 .4979
2 <	135 .4926	120 .4908	154 .4927	120 .4937	135 .5418 #	135 .5054 #	124 .5055 >	124 .5069 #	144 .4992
4 >	124 .4938	144 .4973	144 .4976	144 .4962	144 .5428 #	144 .5058 <	135 .5055 #	135 .5076 #	135 .5001
3	144 .4946	147 .5024 #	147 .5035 #	149 .5016	147 .5445 >	124 .5063 #	82 .5064 #	82 .5114 <	147 .5042
7	107 .4956	149 .5033 #	149 .5039 #	147 .5017	124 .5455 <	147 .5091	147 .5099 <	147 .5116	107 .5043
2 >	109 .4967	134 .5080	134 .5070	134 .5063	107 .5466	107 .5099	109 .5114 #	109 .5119 >	109 .5048
1 <	147 .4969	143 .5088	143 .5090	143 .5064 #	109 .5475 >	109 .5106	107 .5114	107 .5120 >	123 .5061
5	123 .4997 >	124 .5103	107 .5113	139 .5105 <	139 .5481 >	123 .5132 #	139 .5141 >	123 .5147 #	82 .5065
6 #	139 .5023	107 .5106	124 .5114	140 .5107 <	149 .5482 #	139 .5139 >	123 .5145 <	139 .5148	139 .5084
2 #	149 .5024 <	139 .5111	139 .5141	124 .5136 #	123 .5486 #	149 .5143 #	149 .5151 <	149 .5160 >	118 .5106
3 >	118 .5033	140 .5119	140 .5146	107 .5141	140 .5506	118 .5166	106 .5163 >	118 .5162 <	149 .5107
7	106 .5035	109 .5139	109 .5161	131 .5155	106 .5508	106 .5168	118 .5167	106 .5162	140 .5128
9	140 .5060	123 .5158 <	131 .5175	109 .5181	118 .5517	140 .5174	140 .5190	140 .5190	106 .5128
3 <	134 .5141	131 .5168 >	123 .5182	142 .5187	143 .5543	143 .5243	133 .5251	133 .5211	133 .5158
9	143 .5141	106 .5179	106 .5200	123 .5197	134 .5553	134 .5260	143 .5262	165 .5229	165 .5200
5 >	114 .5151	142 .5189	142 .5201	106 .5219	133 .5584 >	114 .5277	165 .5276	143 .5261	143 .5231
4	122 .5182	118 .5208	118 .5239	132 .5239 <	131 .5591 <	133 .5278	134 .5292	161 .5270	188 .5236
2	131 .5198	132 .5251	132 .5255	118 .5255 >	114 .5592 <	131 .5305	188 .5319 #	134 .5281	161 .5249
6	133 .5223	188 .5259	122 .5297	188 .5283	142 .5593 >	122 .5311 >	114 .5321 #	146 .5282	146 .5252

Table 2 (continued)

System 15 35%Ph	System 16 50%Ph	System 17 6%CyPP	System 20 DB-XLB	System 21 DB35MS	System 22 8%PhCS	System 24 Apiezon L	System 26 CNBP#2	System 27 78%CyP
63 .4193	63 .4414	63 .4113	58 .4720	40 .4444	> 63 .4281	98 .3778	93 .4450	64 .3935
74 .4223	74 .4441	94 .4145	102 .4740	121 .4456	< 102 .4292	100 .3787	> 35 .4465	41 .3962
96 .4232	61 .4470	74 .4156	61 .4760	63 .4474	58 .4293	88 .3817	88 .4469	88 .3973
61 .4245	70 .4487	61 .4156	98 .4772	61 .4476	93 .4301	57 .3818	< 95 .4472	63 .3979
40 .4258	94 .4488	98 .4205	63 .4780	80 .4488	98 .4303	58 .3844	121 .4491	58 .3987
94 .4262	96 .4510	< 102 .4212	93 .4781	> 74 .4499	95 .4306	# 84 .3857	67 .4493	93 .3987
70 .4293	76 .4515	> 70 .4218	76 .4784	< 102 .4500	61 .4332	# 91 .3867	58 .4505	150 .4012
76 .4320	40 .4521	121 .4218	95 .4801	76 .4512	74 .4344	67 .3893	91 .4512	74 .4040
> 66 .4340	66 .4530	76 .4226	88 .4807	98 .4517	88 .4352	89 .3935	61 .4535	76 .4101
< 102 .4346	102 .4552	80 .4229	74 .4812	93 .4535	121 .4365	61 .3937	63 .4537	148 .4112
98 .4351	98 .4553	93 .4232	121 .4830	70 .4538	155 .4367	76 .3947	37 .4560	90 .4140
93 .4376	155 .4565	> 66 .4251	70 .4838	155 .4554	91 .4372	63 .3963	76 .4575	91 .4144
155 .4384	93 .4579	< 95 .4254	< 91 .4861	88 .4558	70 .4385	70 .3999	150 .4579	95 .4161
95 .4396	# 95 .4594	88 .4264	> 66 .4863	< 95 .4562	76 .4411	74 .4036	74 .4582	# 92 .4186
88 .4412	# 92 .4600	155 .4291	155 .4867	> 66 .4567	80 .4417	66 .4066	70 .4612	> 35 .4190
92 .4445	88 .4607	91 .4303	80 .4911	91 .4617	66 .4438	55 .4070	# 92 .4629	# 99 .4200
91 .4470	55 .4643	55 .4350	55 .4912	# 92 .4637	92 .4508	152 .4132	# 89 .4634	154 .4215
55 .4471	# 101 .4652	92 .4403	92 .4951	# 110 .4637	55 .4521	56 .4147	152 .4644	80 .4236
101 .4509	# 91 .4655	# 60 .4437	# 84 .4961	55 .4647	84 .4534	121 .4160	> 66 .4656	> 66 .4237
90 .4523	113 .4660	# 56 .4447	> 56 .4963	101 .4681	89 .4559	155 .4186	< 84 .4657	< 101 .4245
113 .4530	90 .4664	90 .4450	# 89 .4968	90 .4681	90 .4564	< 92 .4202	90 .4671	152 .4246
79 .4560	79 .4666	101 .4461	90 .4998	113 .4687	150 .4568	150 .4208	101 .4679	70 .4273
99 .4570	99 .4704	84 .4488	< 101 .4999	< 99 .4718	101 .4575	> 60 .4217	145 .4685	145 .4288
# 56 .4592	111 .4719	# 99 .4502	> 60 .5003	> 56 .4721	# 60 .4605	136 .4234	113 .4711	> 40 .4301
# 60 .4594	# 56 .4744	# 89 .4503	113 .5013	60 .4740	< 113 .4606	145 .4284	99 .4716	113 .4301
119 .4639	# 60 .4744	113 .4508	99 .5039	# 89 .4756	# 56 .4615	113 .4290	55 .4721	< 119 .4307
111 .4656	119 .4752	150 .4558	150 .5048	# 84 .4757	99 .4633	90 .4316	80 .4743	37 .4355
112 .4671	112 .4773	119 .4572	152 .5087	119 .4765	152 .4645	101 .4319	148 .4759	188 .4402
78 .4691	120 .4776	79 .4580	119 .5097	79 .4779	119 .4705	83 .4352	119 .4771	184 .4459
84 .4691	78 .4784	112 .4610	83 .5107	150 .4779	112 .4706	112 .4426	> 56 .4792	108 .4474
108 .4701	108 .4800	108 .4630	112 .5113	112 .4787	145 .4715	99 .4430	< 136 .4794	111 .4484
89 .4715	148 .4835	83 .4649	125 .5121	108 .4805	83 .4736	80 .4435	> 60 .4811	55 .4488
120 .4718	150 .4842	152 .4659	86 .5127	83 .4826	79 .4746	86 .4437	< 83 .4811	116 .4508
150 .4723	84 .4845	78 .4693	108 .5130	111 .4833	108 .4747	125 .4456	154 .4817	112 .4512
148 .4762	# 89 .4855	97 .4701	145 .5138	148 .4835	148 .4774	97 .4469	125 .4822	89 .4529
83 .4768	# 83 .4862	86 .4704	97 .5147	152 .4843	136 .4783	108 .4491	86 .4822	120 .4565
125 .4831	154 .4900	111 .4706	79 .5149	125 .4844	86 .4794	87 .4499	112 .4823	86 .4569
97 .4835	81 .4909	117 .4721	148 .5185	78 .4853	# 117 .4798	119 .4512	108 .4833	125 .4592
152 .4838	125 .4913	145 .4721	116 .5192	86 .4855	# 97 .4799	116 .4604	97 .4857	# 83 .4632
86 .4843	116 .4913	148 .4723	78 .5210	97 .4869	125 .4813	# 85 .4627	116 .4888	# 115 .4637
154 .4844	# 97 .4914	116 .4729	87 .5210	120 .4878	116 .4822	# 117 .4640	# 87 .4907	# 84 .4639
117 .4853	86 .4918	125 .4729	136 .5222	116 .4881	# 115 .4839	# 110 .4643	# 117 .4911	> 60 .4651
116 .4855	# 117 .4918	115 .4736	117 .5230	145 .4891	# 87 .4841	82 .4662	115 .4918	117 .4681
81 .4858	115 .4930	87 .4764	115 .5239	154 .4892	111 .4849	148 .4683	85 .4948	> 97 .4700
115 .4867	152 .4942	120 .4765	111 .5241	# 117 .4919	78 .4857	79 .4702	111 .4955	< 136 .4708
87 .4898	87 .4962	154 .4797	154 .5247	# 115 .4923	154 .4860	115 .4702	151 .4960	> 56 .4721
145 .4915	145 .4993	81 .4799	85 .5250	87 .4931	85 .4895	# 135 .4762	135 .4973	# 139 .4740
85 .4954	< 85 .5010	85 .4799	120 .5284	85 .4967	120 .4917	78 .4763	188 .4977	# 144 .4744
110 .5015	> 77 .5013	136 .4826	110 .5284	81 .4968	> 110 .4941	# 151 .4767	144 .4986	# 151 .4745
151 .5025	< 151 .5043	110 .4874	81 .5302	136 .4997	81 .4949	154 .4845	110 .4994	# 147 .4745
< 136 .5048	# 110 .5044	77 .4931	151 .5350	151 .5022	< 151 .4958	81 .4877	147 .5007	< 135 .4822
> 124 .5052	# 124 .5045	151 .4959	82 .5361	# 135 .5057	135 .4997	144 .4880	120 .5010	> 85 .4833
144 .5078	144 .5084	# 144 .5003	135 .5367	> 77 .5058	144 .5015	111 .4921	184 .5021	140 .4840
135 .5097	107 .5095	> 82 .5010	77 .5383	# 144 .5058	147 .5028	143 .4923	# 139 .5030	87 .4866
107 .5120	> 109 .5098	# 135 .5013	144 .5389	124 .5089	> 82 .5068	149 .4930	79 .5033	149 .4943
109 .5121	# 135 .5103	147 .5027	147 .5419	147 .5097	> 77 .5075	134 .4938	# 149 .5035	79 .4956
147 .5143	# 136 .5106	124 .5046	149 .5428	> 82 .5120	# 149 .5078	147 .4959	140 .5046	143 .5007
123 .5155	165 .5124	139 .5063	< 139 .5449	# 139 .5120	# 139 .5087	77 .4976	143 .5054	133 .5023
106 .5173	123 .5128	107 .5077	> 124 .5454	# 149 .5122	140 .5126	120 .5013	82 .5094	161 .5040
< 139 .5176	# 147 .5137	109 .5078	143 .5458	107 .5125	188 .5133	# 131 .5048	78 .5107	110 .5071
> 118 .5178	# 133 .5137	< 149 .5091	140 .5472	# 109 .5134	124 .5148	140 .5055	134 .5141	168 .5071
# 133 .5197	> 118 .5141	> 123 .5099	107 .5482	# 123 .5138	143 .5163	# 139 .5067	142 .5146	165 .5075
# 149 .5197	106 .5151	140 .5107	# 109 .5495	140 .5150	> 109 .5181	142 .5075	131 .5166	179 .5087
165 .5197	139 .5165	106 .5132	# 123 .5495	106 .5158	107 .5185	132 .5141	< 179 .5181	142 .5098
82 .5213	161 .5170	118 .5134	106 .5515	< 133 .5164	< 134 .5185	124 .5182	> 133 .5188	< 146 .5111
140 .5244	149 .5181	143 .5194	134 .5517	> 118 .5169	123 .5213	107 .5194	> 124 .5193	> 123 .5112
161 .5244	146 .5203	188 .5203	188 .5531	165 .5173	184 .5220	188 .5199	81 .5208	107 .5156
146 .5274	< 140 .5211	# 133 .5208	142 .5533	143 .5175	# 133 .5234	179 .5221	176 .5228	78 .5158
188 .5310	> 82 .5218	# 134 .5216	> 118 .5540	188 .5187	142 .5235	109 .5241	107 .5231	> 124 .5161
143 .5335	127 .5218	114 .5241	# 131 .5544	161 .5205	106 .5236	106 .5258	< 146 .5241	< 176 .5161
127 .5335	188 .5252	142 .5253	# 133 .5546	# 146 .5218	# 131 .5242	# 123 .5258	> 109 .5241	153 .5188

Table 2 (continued)

M #		System 1 100% C1		System 4 50% C8		System 6 50% C8		System 8 50% C18		System 10 DB5MS		System 11 5%Ph		System 12 13%Ph		System 13 20%Ph		System 14 35%Ph
9		*142* .5223	>	122 .5280		114 .5328		122 .5304		122 .5603		*142* .5313		*161* .5323		*188* .5285	<	134 .5295
4		*165* .5295	<	133 .5282		*188* .5339	<	133 .5345		*165* .5605		*165* .5327	<	146 .5328		114 .5301	>	114 .5305
1		146 .5303		114 .5295		133 .5355	>	114 .5347		*188* .5610		*188* .5337		*142* .5330		*142* .5316		*184* .5319
9		*188* .5303		*165* .5340		179 .5390		179 .5375		*161* .5632		146 .5352		131 .5341		131 .5325	#	153 .5324
3	>	105 .5328		179 .5342		*165* .5424		*165* .5419		146 .5636		*161* .5372		122 .5360	>	122 .5337		*168* .5333
2	<	132 .5335		146 .5377		105 .5442		*184* .5420		*184* .5671		*184* .5418		*184* .5396	<	153 .5340	>	122 .5343
6		*161* .5341		*184* .5385		146 .5470	<	146 .5449	#	153 .5687		153 .5421		153 .5400		*184* .5346		*142* .5344
1		153 .5385		*161* .5394		*161* .5492		*161* .5452		*168* .5690	<	132 .5445		*168* .5421		*168* .5357	#	131 .5345
7		*184* .5392		105 .5410		*184* .5492	>	105 .5461	#	132 .5695		*168* .5450		*127* .5433		*127* .5360		*127* .5375
6		*127* .5413	>	153 .5469		176 .5543		176 .5511		105 .5711	>	105 .5454		132 .5522	#	132 .5482	>	105 .5558
9		*168* .5425	<	176 .5472		153 .5577		153 .5552		*127* .5729		*127* .5461		105 .5536	>	105 .5487	#	132 .5559
2		141 .5532		*168* .5474		*168* .5587		*168* .5559	<	179 .5778		141 .5563		141 .5573	#	141 .5493	#	141 .5565
1		179 .5548		141 .5520		141 .5608		*186* .5593	>	141 .5784		179 .5580		179 .5610		179 .5538		179 .5625
5		137 .5608		*186* .5551		*186* .5629		141 .5599		137 .5823		137 .5635		137 .5668		137 .5577		137 .5652
4		130 .5630		130 .5591		130 .5679		130 .5671	<	176 .5837	<	176 .5659		176 .5698	<	176 .5614	<	176 .5718
5		176 .5644		*127* .5607		*127* .5709		137 .5700	>	130 .5844	>	130 .5667		130 .5714	>	130 .5617	>	130 .5727
1	#	138 .5705		137 .5612		137 .5715		164 .5725	#	164 .5875	#	164 .5724		*160* .5755		*160* .5647		164 .5772
2	#	164 .5714		164 .5643		164 .5742		*127* .5762	#	163 .5877	#	163 .5728	#	164 .5756	#	164 .5649	#	163 .5792
4	#	163 .5714	#	163 .5685	#	138 .5794		138 .5773		*160* .5888	#	138 .5733	#	163 .5760	#	163 .5657	#	138 .5797
3		158 .5753	#	138 .5688	#	163 .5797	#	129 .5787		138 .5890		*160* .5747		138 .5780	#	138 .5675	<	178 .5801
9		*160* .5757		129 .5710	#	129 .5802	#	163 .5787		158 .5901		158 .5766		158 .5791	#	158 .5675		158 .5818
8		*186* .5766		*160* .5711		*160* .5818		*160* .5818		*186* .5902		*186* .5768		*186* .5800	<	178 .5677		*160* .5824
6		*126* .5803	<	178 .5736		158 .5863		158 .5845	<	178 .5938		129 .5819		178 .5811		*186* .5696		*186* .5839
5		129 .5804	>	158 .5743		178 .5881		178 .5858	>	129 .5940		*126* .5828	<	175 .5882		175 .5732		175 .5875
7	>	166 .5895		175 .5829		*126* .5991	#	128 .5991		*126* .5972		178 .5832		*126* .5885		*126* .5750		*182* .5896
2	<	178 .5898	<	187 .5876		175 .5994	#	166 .5996	<	175 .5982	<	175 .5886	>	129 .5886		*159* .5752		*159* .5911
4		175 .5970	>	166 .5876	#	166 .6011	<	187 .6005	>	166 .5987	>	166 .5894		*159* .5914		*182* .5764	<	187 .5933
8		*159* .5990		*126* .5890	#	128 .6017		*182* .6026		187 .6008		*182* .5921		*182* .5918	>	129 .5766		*126* .5938
1		187 .6006		*182* .5901		187 .6043		*126* .6047		*182* .6008		187 .5923		187 .5924	<	187 .5768	>	129 .5950
7		*182* .6013		183 .5966		*182* .6080		175 .6063		*159* .6029		*159* .5924		166 .5948	>	166 .5812		183 .5993
3		128 .6030	<	185 .6000		183 .6153		183 .6097		183 .6049		183 .5977		183 .5982	<	183 .5814		*162* .6002
9		*162* .6058	>	128 .6001		185 .6166		185 .6141		*162* .6073		*162* .5981		*162* .5999		*162* .5823		166 .6037
2		183 .6079		*159* .6018		174 .6191		174 .6153		128 .6090		128 .6031		167 .6068		167 .5884		167 .6090
5		167 .6143		174 .6031		*159* .6198		*159* .6213		167 .6118		167 .6053		185 .6114		185 .5932		185 .6197
5		185 .6213		*162* .6064		*162* .6250		177 .6232		185 .6132		185 .6101		128 .6159		128 .6002		128 .6264
1		174 .6296	<	202 .6090		177 .6269		202 .6254		174 .6186		174 .6186		174 .6240		174 .6042	>	174 .6322
6		*181* .6311	>	177 .6097		202 .6295		*162* .6257		*181* .6194		*181* .6200		*181* .6245		*181* .6045		*181* .6326
1		177 .6349		167 .6140		167 .6336		*181* .6293		177 .6222		177 .6246		202 .6294		202 .6069	<	202 .6333
5	>	156 .6412		*181* .6146		*181* .6340	#	171 .6331		202 .6245		202 .6258		177 .6321		177 .6112		177 .6423
2	<	171 .6416	#	171 .6190	#	173 .6370	>	167 .6334		171 .6262		171 .6294		171 .6371	>	156 .6152		*204* .6455
4	<	202 .6469	#	173 .6197	#	171 .6381	#	173 .6339		156 .6284		156 .6309		156 .6381	>	171 .6154		201 .6458
3	>	157 .6472		201 .6231		201 .6460		201 .6402	>	173 .6299	>	173 .6363		201 .6395	<	201 .6155		171 .6477
1		173 .6501		*204* .6324	#	156 .6532		*204* .6502	<	201 .6306	>	157 .6371		*204* .6406		*192* .6156		156 .6497
4		201 .6578		156 .6332	#	157 .6539	<	197 .6546		157 .6319	<	201 .6372		*192* .6415		*204* .6165		*192* .6522
7		*204* .6613		157 .6347		*204* .6575	>	156 .6546		*204* .6323		*204* .6392		173 .6437		172 .6195		172 .6533
2		172 .6631		197 .6366		197 .6623		157 .6554		*192* .6346		172 .6426		172 .6456		173 .6211		197 .6561
8		*192* .6667		200 .6413		200 .6638		200 .6591		172 .6355		*192* .6434		157 .6468	>	157 .6228	<	173 .6597
2		197 .6683		172 .6427		172 .6673		172 .6656		197 .6367		197 .6458		197 .6489	<	197 .6232	>	157 .6598
1		180 .6720		*192* .6466		*192* .6720		*192* .6718	#	180 .6408		180 .6501		180 .6537		180 .6261		180 .6633
2		193 .6767	#	193 .6520	#	193 .6782	#	193 .6762	#	193 .6411		193 .6536		193 .6555		193 .6277		193 .6670
3		191 .6821	#	180 .6528	#	180 .6794	#	180 .6764		191 .6443		191 .6587		191 .6609		191 .6318		191 .6722
4		200 .6878		191 .6584		191 .6858		191 .6829		200 .6486		200 .6640		200 .6700		200 .6411		200 .6847
6		*169* .6980		170 .6752		170 .7016		170 .6988		*169* .6572		*169* .6732		*169* .6788		*169* .6467		*169* .6953
2		170 .7075	>	190 .6823		190 .7111		190 .7089	#	170 .6614		170 .6826	<	198 .6914		198 .6556		198 .7072
3		190 .7120	<	198 .6824		*169* .7117	#	198 .7099	#	190 .6618		190 .6842	>	190 .6920		190 .6587	<	199 .7133
8		198 .7256		199 .6833	#	198 .7140	#	199 .7105		198 .6647		198 .6894		170 .6944	<	199 .6609	#	170 .7140
1		199 .7292		*169* .6847	#	199 .7150		*169* .7173		199 .6671		199 .6920		199 .6970	>	170 .6610	#	190 .7151
2	#	196 .7372		196 .6936		196 .7268		196 .7209	#	203 .6716	#	203 .6983		203 .7023		203 .6652	#	203 .7210
1	#	203 .7372		203 .6965		203 .7303		203 .7248	#	196 .6718	#	196 .6986		196 .7041		196 .6670	#	196 .7214
5		189 .7537		208 .7128		208 .7500		208 .7432		189 .6841		189 .7147		189 .7227		189 .6816		189 .7450
1		195 .7736		195 .7196		195 .7537		195 .7477		208 .6916		208 .7294		208 .7351		208 .6912		208 .7547
3		208 .7802		189 .7228		189 .7580		*207* .7577		195 .6929		195 .7308		195 .7438		*207* .7005		*207* .7671
3		*207* .7917		*207* .7271		*207* .7671		189 .7586		*207* .6980		*207* .7386		*207* .7455		195 .7008		195 .7728
1		194 .8075		194 .7550		194 .7965		194 .7925		194 .7089		194 .7538		194 .7633		194 .7143		194 .7922
2		205 .8169		205 .7619		205 .8050		205 .8022		205 .7117		205 .7600		205 .7671		205 .7168		205 .8004
1		206 .8652		206 .7887		206 .8368		206 .8303		206 .7346		206 .7948		206 .8036		206 .7459		206 .8394
3		*209* .9110		*209* .8124		*209* .8659		*209* .8583		*209* .7622		*209* .8293		*209* .8374		*209* .7728		*209* .8745
#		35		23		25		39		35		35		22		30		41
<,>		20		24		11		11		17		25		17		25		22
Sum		55		47		36		50		52		60		39		55		63

Table 2 (continued)

System 15 35%Ph		System 16 50%Ph		System 17 6%CyPP		System 20 DB-XLB		System 21 DB35MS		System 22 8%PhCS		System 24 Apiezon L		System 26 CNBP#2		System 27 78%CyP	
153	.5338	153	.5256	131	.5256	*184*	.5582	# 134	.5221	> 118	.5250	# 118	.5333	123	.5242	# 134	.5228
168	.5353	*168*	.5267	*165*	.5260	122	.5586	*142*	.5235	*165*	.5290	# 122	.5334	*165*	.5256	# 131	.5233
114	.5354	114	.5279	*184*	.5272	*165*	.5588	*184*	.5237	146	.5308	< 133	.5365	132	.5265	> 109	.5235
134	.5364	*143*	.5287	146	.5272	146	.5599	131	.5254	114	.5328	*184*	.5368	*106*	.5269	*186*	.5247
184	.5375	134	.5305	*161*	5291	114	.5609	*168*	.5257	*161*	.5339	176	.5391	*186*	.5270	*106*	.5272
142	.5391	*184*	.5305	122	5297	*161*	.5618	153	.5263	< 179	.5346	114	.5429	*161*	.5273	118	.5322
122	.5397	122	.5320	153	.5338	# 153	.5646	114	.5271	> 132	.5348	*186*	.5441	*168*	.5280	*81*	.5339
131	.5407	*142*	.5332	*168*	.5355	*168*	.5647	122	.5278	> 122	.5381	*165*	.5450	> 118	.5293	*182*	.5356
141	.5522	131	.5345	132	.5408	# 132	.5649	*127*	.5330	< 153	.5384	146	.5490	< 153	.5293	82	.5372
105	.5564	141	.5401	*127*	.5442	179	.5701	# 141	.5378	*168*	.5398	105	.5526	77	.5317	*204*	.5426
132	.5586	105	.5455	105	.5443	106	.5727	# 132	.5382	176	.5422	*161*	.5527	# 114	.5360	178	.5431
179	.5610	# 137	.5486	179	.5478	141	.5734	179	.5391	141	.5487	*168*	.5598	# 122	.5365	> 114	.5447
137	.5626	# 132	.5491	141	.5494	176	.5756	105	.5415	*127*	.5508	# 141	.5609	141	.5382	< 175	.5449
130	.5671	< 179	.5493	< 176	.5549	137	.5781	137	.5433	*186*	.5509	# 153	.5612	> 137	.5425	202	.5464
< 176	.5691	178	.5512	> 137	.5552	*127*	.5787	176	.5449	105	.5515	130	.5691	< 178	.5428	137	.5522
160	.5694	> 130	.5521	130	.5598	*186*	.5803	130	.5472	137	.5550	# 164	.5729	*182*	.5440	> 141	.5559
# 163	.5700	*160*	.5525	*186*	.5651	130	.5811	> 164	.5480	130	.5575	# 137	.5738	175	.5459	< 201	.5560
# 164	.5702	*159*	.5529	# 163	.5654	164	.5826	< 178	.5481	178	.5602	129	.5771	130	.5467	# 187	.5581
< 178	.5704	# 163	.5534	# 138	.5658	138	.5857	*160*	.5495	# 164	.5624	# 138	.5819	> 164	.5493	# 183	.5586
# 158	.5740	# 164	.5539	# 164	.5664	163	.5867	*186*	.5497	# 163	.5625	# 163	.5830	< 187	.5493	> 122	.5608
# 138	.5740	< 176	.5560	*160*	.5674	*160*	.5869	163	.5504	138	.5648	< 178	.5836	> 105	.5516	< 132	.5613
159	.5753	# 158	.5565	158	.5680	> 129	.5879	138	.5515	*160*	.5665	*160*	.5845	138	.5518	197	.5646
175	.5772	< 175	.5568	178	.5710	< 178	.5879	> 158	.5523	175	.5666	158	.5905	< 183	.5523	> 77	.5747
186	.5796	# 138	.5575	> 129	.5757	158	.5894	< 175	.5525	> 158	.5678	*127*	.5954	< 202	.5535	< 130	.5753
126	.5807	*126*	.5591	< 175	.5762	175	.5918	*182*	.5537	< 187	.5688	175	.5969	> 163	.5539	*160*	.5818
182	.5807	187	.5603	*182*	.5780	*182*	.5921	187	.5555	*182*	.5690	< 187	.6013	# 158	.5554	# 138	.5843
187	.5811	*162*	.5604	> 166	.5797	187	.5938	129	.5571	129	.5713	> 128	.6028	*160*	.5556	# 158	.5856
162	.5843	*182*	.5608	< 187	.5798	183	.5980	*159*	.5585	< 183	.5755	*182*	.6043	# 129	.5558	# 164	.5857
129	.5856	*186*	.5639	*126*	.5826	166	.5989	183	.5591	> 166	.5763	166	.6080	*204*	.5575	163	.5890
183	.5868	183	.5649	*159*	.5838	*126*	.6027	*126*	.5624	*126*	.5847	# 174	.6121	201	.5589	185	.5933
# 166	.5909	167	.5662	183	.5847	*159*	.6031	166	.5631	> 185	.5853	# 183	.6135	185	.5627	*181*	.5952
# 167	.5911	129	.5672	*162*	.5904	> 128	.6065	*162*	.5638	*159*	.5854	# 185	.6140	*127*	.5636	105	.5974
185	.5996	166	.5689	167	.5969	< 185	.6066	> 167	.5685	< 202	.5860	202	.6180	< 197	.5640	*159*	.6003
< 202	.6127	185	.5748	> 128	.5980	*162*	.6067	< 185	.5686	*162*	.5901	177	.6234	> 166	.5647	*127*	.6004
# 181	.6134	*192*	.5837	< 185	.5984	174	.6093	< 202	.5749	< 174	.5904	*126*	.6247	> 174	.5647	166	.6016
# 174	.6135	202	.5844	181	.6062	167	.6118	> 174	.5755	> 128	.5911	173	.6313	*181*	.5676	129	.6050
> 128	.6139	# 181	.5861	174	.6079	*181*	.6130	*181*	.5767	181	.5928	181	.6341	177	.5721	174	.6123
192	.6173	# 174	.5867	202	.6095	202	.6139	128	.5768	201	.5944	> 171	.6356	*159*	.5744	200	.6149
177	.6217	128	.5889	177	*.6130*	177	.6164	201	.5817	< 177	.5958	< 201	.6363	> 128	.5748	*162*	.6178
< 201	.6229	172	.5909	> 171	.6172	< 201	.6198	*204*	.5817	*204*	.5965	*159*	.6383	< 171	.5749	177	.6247
204	.6232	> 156	.5919	< 201	.6178	> 171	.6199	177	.5821	> 167	.5972	*162*	.6421	200	.5775	< 171	.6270
> 156	.6240	< 201	.5925	*204*	.6182	*204*	.6204	*192*	.5848	> 171	.6022	*204*	.6502	*162*	.5783	> 167	.6274
> 172	.6241	> 177	.5928	156	.6230	173	.6224	171	.5856	< 197	.6028	> 167	.6515	173	.5803	*192*	.6420
171	.6267	*204*	.5930	> 173	.6251	197	.6259	> 172	.5876	173	.6081	# 200	.6525	167	.5839	173	.6445
> 180	.6318	# 171	.5969	< 197	.6255	> 156	.6289	< 197	.5876	< 200	.6171	# 197	.6537	172	.5906	172	.6476
< 197	.6321	# 193	.5972	> 157	.6298	< 172	.6290	< 173	.5887	> 172	.6176	# 157	.6718	*126*	.5921	< 208	.6528
> 157	.6322	> 180	.5973	< 172	.6305	157	.6309	156	.5889	156	.6190	# 156	.6719	*192*	.5961	> 128	.6539
# 193	.6330	> 157	.5989	*192*	.6315	*192*	.6314	# 180	.5928	*192*	.6216	172	.6770	180	.5962	180	.6575
# 173	.6333	< 197	.5996	180	.6374	180	.6345	# 193	.5933	157	.6243	*192*	.6857	193	.6000	*207*	.6642
191	.6376	# 173	.6019	193	.6415	193	.6360	> 157	.5936	180	.6255	# 193	.6888	< 191	.6022	198	.6653
169	.6522	# 191	.6022	> 191	.6453	200	.6378	191	.5966	193	.6267	# 180	.6899	> 156	.6027	191	.6671
200	.6546	*169*	.6098	< 200	.6463	191	.6402	200	.6015	191	.6326	191	.6964	157	.6057	193	.6700
198	.6641	200	.6168	*169*	.6686	> 170	.6558	198	.6116	# 198	.6462	170	.7113	# 198	.6066	199	.6764
< 199	.6705	198	.6189	170	.6711	< 198	.6560	*169*	.6137	# 199	.6469	# 198	.7184	# 199	.6071	196	.6789
> 190	.6708	199	.6246	< 198	.6722	199	.6567	199	.6149	170	.6520	# 199	.7185	< 208	.6103	*126*	.6812
< 203	.6748	190	.6258	> 190	.6724	190	.6591	190	.6179	# 196	.6540	190	.7254	> 196	.6108	203	.6814
> 170	.6753	203	.6282	199	.6758	*169*	.6613	> 170	.6187	# 203	.6550	196	.7308	203	.6133	156	.6828
196	.6772	> 170	.6307	# 203	.6812	196	.6614	< 203	.6190	> 190	.6553	203	.7362	*207*	.6159	157	.6916
189	.6905	< 196	.6310	# 196	.6815	203	.6621	196	.6197	*169*	.6565	208	.7451	170	.6185	170	.7250
208	.7031	189	.6380	189	.7038	208	.6776	208	.6348	208	.6644	*169*	.7480	190	.6243	190	.7280
207	.7134	208	.6492	208	.7058	189	.6821	189	.6358	*207*	.6730	195	.7588	195	.6359	195	.7506
195	.7173	*207*	.6577	*207*	.7140	*207*	.6841	*207*	.6418	195	.6814	*207*	.7634	*169*	.6486	*209*	.7621
194	.7259	195	.6618	195	.7151	195	.6842	195	.6459	189	.6865	189	.7874	189	.6536	189	.7793
205	.7274	# 194	.6651	194	.7388	194	.6977	194	.6558	194	.7082	194	.8203	194	.6596	*169*	.7905
206	.7595	# 205	.6653	205	.7457	205	.7049	205	.6579	205	.7156	205	.8345	*209*	.6647	194	.7975
209	.7887	206	.6899	206	.7749	206	.7216	206	.6761	206	.7294	206	.8647	205	.6676	206	.8012
no PCB 77		*209*	.7117	*209*	.7990	*209*	.7383	*209*	.6926	*209*	.7397	*209*	.8946	206	.6685	205	.8085

	System 15	System 16	System 17	System 20	System 21	System 22	System 24	System 26	System 27
#	33	47	25	12	30	28	51	24	28
<,>	19	17	30	22	26	32	13	29	30
Sum	52	64	55	34	56	60	64	53	58

eluting closely after a tailing major peak). This criterion is less exacting than one requiring baseline separation of peaks, which produces the most accurate quantitation. An Excel 4.0 spreadsheet was programmed to predict congener coelutions and separations in each system based on the former, less strict, criterion. These are indicated in Table 2 by enclosing the coeluting congener numbers in a box. The potential for coelution with congeners not significantly present in Aroclors will not affect quantitation of significant Aroclor components *in an Aroclor distribution which has not been subjected to a dechlorination process which produces non-Aroclor congeners*. MS detection can often enable separate quantitation of coeluting homologs of different chlorine number in Aroclors. In front of the bold-faced *Aroclor* congener numbers in the predicted coelution boxes for each system in Table 2, the symbol # indicates coelution with another *Aroclor* congener of the same chlorine number, unresolvable by either ECD or MS detection. The symbols < or > indicate respectively the higher or lower homologs in a coeluting group which may possibly be quantitated using MS detection if the relative proportions are suitable. The totals for each system of *Aroclor* congeners flagged by #, either < or > (possibly measurable by GC-MS), and by all 3 symbols (not resolvable by ECD or ELCD) are summarized for each system in Table 1A. The elution time of PCB 209 displayed in the last column of that table is an indication of the system's total analysis time.

Discussion

There were no close elutions or inversions of expected elution order in the 30 mixtures of 6 or 7 congeners on all systems except for highly polar phases in systems 23, 26, and 27. Mass spectral information was necessary to complete congener assignments to peaks for those three, whose radical variations from other phases in the elution orders of PCBs are illustrated by the elution of some congeners *after* PCB 209. Note their much higher relative retention of non-*ortho*-chlorine-substituted congeners 77, 81, 126, 169 etc. Phases of this type may prove useful as the second column in a method employing the newly developed technique of comprehensive 2D-HRGC for CQCS PCB analysis [29], and the database illustrated by Table 2 enables facile predictions of the likely congener resolutions achievable with different pairs of columns in such a method.

Changes of the parameters of column dimensions, stationary phase film thickness, carrier gas (H_2 vs He) pressures and flow rates, and column temperature programs, can all affect both the calculated relative retention times (RRTs) and the resolvability of congeners [6]. Therefore the congener resolvability flags in Tables 2 and 1A serve only as a guide to what might be achievable with a particular column, and congener identification should not be attempted solely by matching the listed numerical values of RRTs. The size of the percentage difference between the RRTs of congener pairs to be resolved is the best measure of the suitability of a particular column for the task. As an example, analysts seeking to measure the trace amounts of important non-*ortho*-substituted congeners in Aroclors without preseparation might select system 17 to measure PCB 77 (separated on either side from PCB 110 by 1.15% and PCB 151 by 0.57%). When a duplicate column was purchased and PCBs were analyzed under closely similar conditions, non-*ortho*-substituted PCB 81 eluted after PCB 85, and PCB 77 moved closer to PCB 151, being barely resolvable by only 0.23%). Such variability is an unfortunate feature of cyanopropyl-substituted silicone phases such as systems 17, 18, and 27 [9]. In system 20, PCB 77 was predicted to be just resolvable from PCB 144, but the separation of only 0.11% resulted in an inability to measure it in Aroclors 1254, 1260 or 1262, where its peak merged with the much higher levels of PCB 144. In lower Aroclors, the much smaller amounts of PCB 144 permitted measurement of PCB 77 with system 20, after subtraction of the small amount of interfering 2-chlorine-loss fragment signal from PCB 144. System 20 elutes PCB 126 0.67% after minor Aroclor PCB 166, while it would coelute with PCB 159, which is not detected in Aroclors, and which could be confirmed as absent by MS monitoring of its more massive molecular ion. Table 2 facilitates rapid evaluations in this fashion for different lists of priority congeners to select the best column(s) for detailed study and method optimization. Its complete congener listings are especially valuable for designing CQCS PCB analyses which must deal with "non-Aroclor congeners" derived from processes such as Aroclor dechlorination.

The complete 27 column database contained 4 cases of more than one column of a given stationary phase structure (3 DB-1, 4 SPB-Octyl, 2 CP-Sil5-C18, and 2 CNBP). Of these Table 2 displays only Systems 4 and 6 for SPB-Octyl. A close comparison of this pair illustrates both that the values of RRTs differ substantially, as expected for different column dimensions and chromatographic conditions, and that there are small but significant differences in the exact elution orders and resolvabilities of some congener pairs (e.g. PCBs 70 and 74). Similar differences were observed between systems 8 and 9, and between 23 and 26, while the 3 polydimethylsiloxane phases (systems 1, 2, and 3) behaved more reproducibly. These observations reinforce the recommendation of the database primarily as a guide to column selection prior to precise calibration of the selected system with congener standards in the analyst's lab.

The most suitable column for a PCB analysis will depend on the application and the congeners which must be measured. For CQCS analyses to most completely characterize congener distributions in Aroclors, pairs of columns employed by 3 labs proved particularly comprehensive; namely, GE-CRD (systems 1 or 2 and system 4), HWRIC (systems 3 and 6 [same phases as 1st pair]), and Chrompack (systems 8 and 12). Two phases were particularly effective for CQCS analyses when used singly with MS-SIM detection to permit quantitation of coeluting homologs of differing chlorine number. The DB-XLB column (system 20) is seen in Table 1A to have an unusually low number of predicted Aroclor coelutions. A close inspection in Table 2 of those in which different homologs coelute, and reference to congener weight percents in Table 2 of the 2nd paper [2], reveal that in most cases the minor component is the heavier congener, thus measurable by MS without interference, and producing negligible $M^+ - 1$ Cl fragment ion to interfere with the major component. As mentioned above, important congener 126 is well resolved on this column. It permits measurement of 21 of 28 microbial *meta*- and *para*-dechlorination products [30] different or elevated from congeners in Aroclors 1254 or 1260, even in the presence of lower Aroclors. It resolves 10 of 12 coplanar non- or mono-*ortho*-chlorine substituted PCBs [31]. While the predicted number of coelutions in Table 1A would not flag the HT-8 column (system 22) as superior to others, Larsen et al. [12] have published detailed Aroclor resolution information, mainly confirmed in this study, which suggests that it is particularly suitable for CQCS analyses which require maximum resolution of sets of priority congeners [6, 7] from other Aroclor congeners. In particular HT-8 resolved important priority hexachlorobiphenyl congeners 153 from 132, and 138 from 163, 164 while DB-XLB did not. Again the choice depends on the application. Both these phases were developed to have very low bleed over a wide temperature range for employment in GC-MS systems.

Compare in Table 1A the isomer resolution performance between systems 14 and 15, which used closely similar stationary phases, but different column dimensions and chromatographic conditions. System 15 is predicted to resolve 8 more isomers plus 3 more different homolog pairs at the cost of a more than 3-fold longer analysis time. A similar comparison among systems 1, 2 and 3, and among systems 4, 5, 6 and 7 is likewise instructive for evaluating performance vs analysis time tradeoffs.

Based on the resolvability of Aroclor congeners summarized in Table 1A and historical application to CQCS PCB analyses, 12 of the 20 phases were nominated as most important for this application, and their systems are enclosed in boxes in the table. Starting with systems 1, 4, 11, and 20, Aroclor congeners (bold in Table 2) and non-Aroclor congeners were separately assigned to a minimum number of mixtures allowing substantial separation in elution times in each mixture for all 4 columns. A spreadsheet macro program was developed to rapidly calculate the separations in W@½H units of congeners assigned to each mixture for all systems in the database. Congeners were then iteratively reassigned among the mixtures to minimize the number of "close elutions", (defined as pairs of congeners within a mixture predicted to elute within 6 W@½H units on any of the 12 selected phases). This separation was chosen to allow for the amount of variation in relative elution times for congeners observed among different systems employing the same stationary phase. To minimize the number of mixtures required, some minor Aroclor congeners were assigned to the non-Aroclor mixtures, and some non-Aroclor congeners to the Aroclor mixtures. Eventually 5 mixtures of 144 mainly Aroclor congeners and 4 mixtures of 65 mainly non-Aroclor congeners were defined with an acceptably low number for the 12 phases of residual "close elutions", which are tabulated in Table 1A. To have eliminated all close elutions for the 12 phases would have required more than double the number of mixtures. When used with the elution information in Table 2, injection of the first 5 mixtures on an HRGC system would enable assignment and quantitative calibration for significant Aroclor congeners, while injection of the additional 4 mixtures would complete the process for all 209 congeners. Initial column "M #" in Table 2 associates the assignment to mixture number of each congener with its IUPAC number listed in the adjacent column for system 1. Solutions of the 9 calibration mixtures formulated according to this scheme are available from AccuStandard, Inc (New Haven, CT, USA), together with elution orders of the congeners in each mixture on each of the stationary phases in this retention database (also included in supplemental material, see below).

The database provides a rich trove of retention data to thoroughly test QSAR-based HRGC retention prediction algorithms for PCB congeners [6, 14, 23]. Its availability renders such programs largely unnecessary for CQCS PCB analyses on the stationary phases reported. If sufficient predictive accuracy can be demonstrated, the algorithms may be useful for predictions on systems not in the database. The need in some instances for extremely accurate predictions to identify resolution and elution order for close pairs suggests that use of the 9 congener calibration mixtures with MS-SIM detection might be more efficient for this purpose, as well as providing absolute quantitative standards. However, the lack of reference retention orders for the mixtures on these systems would probably require injections of some additional single congener standards to resolve uncertainties in assignments. If adequately validated against the PCB retention database, and applied to compounds of similar functionality such as chlorinated dioxins, dibenzofurans, diphenyl ethers, etc., the predictive programs may find their greatest usefulness in circumstances where complete congener standard sets are still not readily available.

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